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Modelling and Simulation of a Gas-to-Liquid Technology Using Fischer-Tropsch Process

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Abstract
Gas-to-liquid (GTL) technology is a process that involves the conversion of natural gas into liquid hydrocarbons, which can be further processed into fuels and other hydrocarbon-based products. This process is very useful where gases are available in abundant quantities. It has been discovered that the process has not been well established, and, therefore, it is one of the areas being looked into seriously by process engineers. In order to contribute to the success of the development of this technology, this research work was studied with the aim of modelling, assessing and optimizing a gas-to-liquid plant based on Fischer Tropsch process towards ensuring a safe and economically viable system. This was achieved through the use of Aspen HYSYS process simulator. The natural gas used as the feed was taken to contain the following components: methane, ethane, propane, n-butane and nitrogen. The model of the gas-to-liquid was developed by picking the pieces of equipment involved in the process from the object palette of the process simulator, placing them on the modelling sheet and joining them together. Thereafter, the operating parameters of the process were inputted into the appropriate places in the model. The developed model was simulated with Peng-Robinson as the fluid package that was employed to estimate the thermodynamic properties. The results obtained from the simulations showed that the natural gas was converted to liquid hydrocarbons that can be processed further for the production of other desired products like gasoline, kerosene, diesel and wax. Therefore, the production of liquid from natural gas has been achieved successfully with the aid of Aspen HYSYS.

Keywords: Gas-to-liquid, Fischer-Tropsch, syngas, reformer, Aspen HYSYS.

1. Introduction

Natural gas can be described as a mixture of hydrocarbons with varying quantities of non-hydrocarbons that exist in either the gas phase or in solution with crude oil in underground reservoirs. Natural gas comes from three types of wells: oil wells, gas wells and condensate well. There are two main primary sources of natural gas: associated gas and non-associated gas. Associated gas is usually found in the oil wells either dissolved in the oil or as a gas cap above the oil. Non-associated gas is usually found in gas and condensate wells. They usually occur alone (Shah and Durr, 2007). The amount of heat produced during the combustion of natural gas is called the heating value, and it can be measured in British thermal unit (BTU) (Ubani and Goodness, 2016).

Nigeria is one of the top ten countries with the largest gas reserves (associated and non-associated) and is the largest in Africa with an estimated gas reserve of over 166 trillion standard cubic feet (TCF) (NAPIMS, 2018). Nigeria has an economy that relies on both crude oil and natural gas for its domestic and international market. Oil and gas exploration began in Nigeria in 1908 with the first discovery made at Oloibiri village at Bayelsa state in 1956 by the Royal Dutch shell. During the early days of oil production, associated gas was discovered and was treated as an incidental product and was completely flared until 1963 when the development of natural gas started with the sale of natural gas at Ughelli and Aba to companies around the gas fields (Udok and Akpan, 2017). However, gas flaring was still at a high rate until 1999 when gas utilization schemes and regulatory intervention reduced the flaring. Despite all these, Nigeria has been ranked the sixth largest gas flaring country globally according to the World bank's global gas flaring reduction partnership ranking. According to the Nigerian gas flare tracker, between March, 2012 and October, 2019, 1.5 billion Mscf has been flared with a CO_2 emission of 78.2 million tonnes. The gas flared is valued at 5.2 billion USD and the potential power generation from this would have been about 147.2 thousand GWh. According to the satellite data estimates from Nigeria's environment ministry, over 313 million standard cubic feet of gas is flared annually by oil companies in Nigeria (Richard-Koko, 2020).

The term "Gas flaring" can be defined as the combustion of gas in an open flame that burns continuously at the top of the flare stack at oil or gas production sites. Gas venting, on the other hand, is the intentional discharge of unburned gas into atmosphere; this is usually done to maintain safe working conditions during operation or due to surplus gas which have no export route or market value. Flaring gas wastes a valuable energy resource, which could be used to generate revenue and support economic growth and progress, if utilized. It also affects the environment negatively as it contributes to climate change by releasing millions of harmful gases into the atmosphere (Richard-Koko, 2020). Gas flaring has posed some serious issues over the past years, hence the need to search for an alternative to flaring has led to the development of Liquefied Natural Gas (LNG) and Gas-to-Liquid (GTL) technologies, which aim at reducing flaring by conversion of the gas for storage.

The Gas-to-Liquid (GTL) technology was invented in 1923, when two German scientists, Franz Fischer and Hans Tropsch, discovered the catalytic conversion of carbon monoxide and hydrogen (synthesis gas) into synthetic hydrocarbons. Gas-to-Liquid is a process in which natural gas is converted to liquid hydrocarbon. The GTL process involves feeding natural gas (methane) into a reformer or generator where it is converted into synthesis gas (a combination of carbon monoxide and hydrogen). It excludes the production of liquefied natural gas (LNG), but includes the conversion of gas to methanol, liquid fuels, and petrochemicals, being the most common applications. In other words, GTL is a process for converting natural gas into synthetic fuel, which can be further processed into fuels and other hydrocarbon-based products (Richard-Koko, 2020).

According to the information obtained from literature, various researchers have worked on topics related to the subject matter of this work. Among them are Bao (2008) who provided a technoeconomic analysis of GTL process and also identified optimization and integration opportunities. After the analysis and integration, it showed that using a feed designed for 128,000 bbl/d, at least 68,000 bbl/d is needed to keep the process profitable with a return on investment (ROI) of 5.1%. Also, 884 million $/yr was saved from heat integration, 246 million$/yr from heat cogeneration and 22 million$/yr from waste management. Kim et al. (2008), using Aspen HYSYS, conducted a study to find out he optimum parameters for the production. The reactions are governed by Soave-Redlich-Kwong (SRK) equation. The auto thermal reformer was used for the syngas production and a cobalt based catalyst was used for the slurry bubble reactor. The syngas composition and operating temperature of the reactor were varied and the optimum operating parameters of the GTL process were H_2/CO ratio of 2 and a temperature of 255 ˚C. The results of the simulation, when compared with the actual experimental results, were found to be in reasonabe agreement with each other. Lee (2010), with the aid of Aspen HYSYS software and MATLAB, conducted a study to optimize Fischer Tropsch (FT) Plants in order to produce gasoline and gas oil. This was done by investigating the benefits of recycling and co-feeding of unconverted gas, undesired compounds, and lighter hydrocarbons over iron-based catalysts in order to save on capital and operating costs. It involved the development of FT models for both two-phase and three-phase reactors. The kinetic parameters for these models were estimated using optimization carried out with the aid of MATLAB fitting to experimental data, and these models were applied to Aspen HYSYS flowsheets in order to simulate nine different Fischer-Tropsch plant designs. The proposed FT reaction mechanisms were interpreted qualitatively by both Driving Force Analysis (which shows analysis of each compound necessary for the Fischer-Tropsch reaction and mechanism, and understood the influence of selectivity products on the reaction) and via reactor modelling. MATLAB was used to accomplish the study of the effects of some parameters such as size of catalyst and reactor. The results revealed that the plants involving recycling and co-feeding produced higher quantities of gasoline and gas oil. The proposed heuristic regarding the economic scale of the optimized model was evaluated and the capital cost of the optimized FT plant reduced by 30% when compared with the real FT plant proposed by Gerard. This shows that the recycling and co-feeding to FT reactor plant was the best efficiency to produce both gasoline and gas oil. Knutsen (2013) investigated the operation performance and optimization of a GTL plant excluding the upgrading unit with the aid of Honeywell's Unisim design R400 and the selected fluid package was Peng-Robinson. The autothermal reformer and multi tubular flow reactor were simulated together with a cobalt catalyst. A feed designed for 17000 bbl/d was used for the simulations. After the simulations, the optimized process produced 19000 bbl/d of syncrude with carbon efficiency of 82.41% and a thermal efficiency of 65.93% without the inclusion of economics. After considering economics, the crude was reduced to 18620 bbl/d, carbon and thermal efficiencies were 77.25% and 61.77% respectively. After comparing the production cost and revenue, it indicated a good economic environment for the GTL process. Otaraku and Vincent (2015) carried out a technical analysis aimed at element incorporation, structure generation and optimization of a gas to liquid plant. The plant was limited to syngas production and the Fischer Tropsch reactor, thereby excluding air separation unit, desulphurization unit and the product upgrading unit. This was done with aid of Aspen HYSYS with Peng Robinson as the fluid package. The base case was analysed for both carbon and thermal efficiency and product flow to the upgrading unit, and the optimised values were 82.41%, 65.93% and 19940 bbl./d respectively. Rafiee and Panahi (2016) investigated the simulation of a GTL plant with a multistage cobalt-based Fischer-Tropsch reactor and interstage product separation was also considered with the aid of Aspen HYSYS process simulator. The FT reactor is a slurry bubble column type and was modelled as continuous stirred tank reactor (CSTR). The total volume of the FT reactors was fixed at 2000 m^3 which was the same as the one used in the Sasol Oryx Plant. It was discovered that the more the number of stages, the higher the rate of wax production which were given as 77753, 78948, and 79216 kg/h for the single, two and three stage FT reactor respectively of the same volume of 2000 m^3. Sectioning of the Fischer-Tropsch reactor increased the chain growth probability inside the reactor, and this resulted in a higher production of wax. Chinedu et al. (2019) considered two cases during the simulation of the GTL plant with the aid of Honeywell's Unisim software and Peng-Robinson as the fluid package. The first case involved feeding oxygen as a reactant into the ATR for the production of syngas while the second case fed CO_2 in place of oxygen as a reactant for the production of synthesis gas. The choice of CO_2 was influenced by its cheap availability and its ability to be recycled from purge gas and reused, thereby reducing pollution. Technoeconomic analysis of the two cases were performed. It was revealed that the proposed CO_2 method gave a lower H_2/CO ratio of 2.17 as compared with O_2 method which gave a ratio of 2.21. A carbon efficiency of 77.68% for the base case and 92.17% for the proposed method indicated a higher efficiency for the proposed case. Liquid yield also indicated the proposed method has a higher yield of 5730 bbl/d in comparison to the base case with a yield of 5430 bbl/d, thus representing an increase in the product yield by 5.5%.

In order to contribute to the development of the GTL process, this work has been carried out to model and simulate a gas-to-liquid (GTL) plant using Fischer-Tropsch technology that will ensure a safe, environmentally friendly and economically viable process with the aid of Aspen HYSYS process simulator.

2. Methodology

2.1 Process Selection

There are various ways of modelling a GTL plant, all of which involves the three major sections, viz. production of synthesis gas, Fischer-Tropsch reaction to produce long chain hydrocarbons and upgrading of products to get the desired products. The accuracy of the results depends on the method chosen. There are various technologies available for the production of syngas, a feed of natural gas is fed to the pre-reformer which is installed before the main reformer (the auto-thermal reformer). This was best suited for the process after comparison with the other known reformers. For the Fischer-Tropsch reaction, the Low Temperature Fischer Tropsch (LTFT) reactor was used for the process. This was chosen with respect to our desired product.

During the modelling and simulation of this work, some assumptions were made and they include:

(i) isothermal
(ii) steady-state,
(iii) using pre-treated natural gas to remove sulphur.
(iv) taking air to be composed of only oxygen.

2.2 Model Development and Steady state simulation

In a typical GTL plant, there are three sections which include the syngas production, the Fischer-Tropsch reactions and the product upgrade. The GTL plant consists of one distillation column (for the products), two heat exchangers, four heaters, five reactors (pre-reformer, auto-thermal reformer, two water gas shift reactor and Fischer-Tropsch reactor respectively). The conceptual model was actualized with the Aspen HYSYS software in accordance with existing technologies.

2.3 Modelling of Gas to Liquid Plant

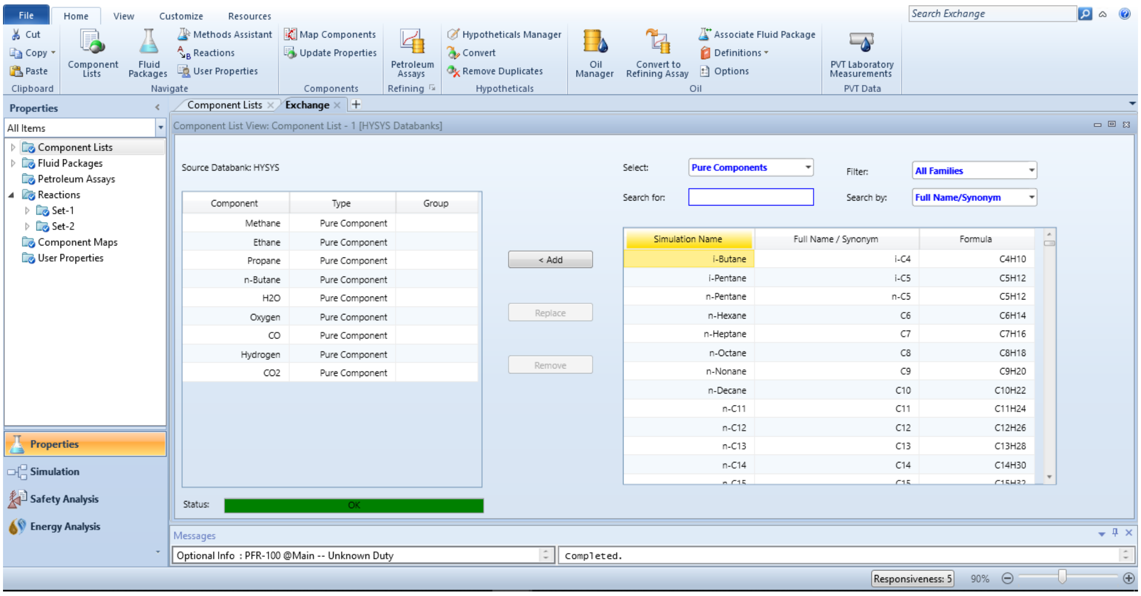
The process model was developed and simulated using the Aspen HYSYS V11 (Aspen, 2019) via the steps outlined thus.

2.3.1 Component Selection

The chemical components involved in the process were chosen from the Aspen HYSYS database. To select the components,

i. a new model was opened in Aspen HYSYS V11,
ii. under ‘Components Lists’ in ‘Properties’ environment, ‘Add’ was clicked, and
iii. the necessary components were selected. All hydrocarbons with more than one carbon atom were added as n-type hydrocarbons. Other components added include water, oxygen, carbon monoxide, hydrogen and carbon dioxide

Figure 1 shows the pictorial representation of the selection of components in Aspen HYSYS:



Component List View: Component List - 1 [HYSYS Databanks]

Source Databank: HYSYS

Component	Type	Group
Methane	Pure Component	
Ethane	Pure Component	
Propane	Pure Component	
n-Butane	Pure Component	
H2O	Pure Component	
Oxygen	Pure Component	
CO	Pure Component	
Hydrogen	Pure Component	
CO2	Pure Component	

Status: OK

Select: Pure Components
Filter: All Families
Search for:
Search by: Full Name/Synonym

Simulation Name	Full Name / Synonym	Formula
i-Butane	i-C4	C4H10
i-Pentane	i-C5	C5H12
n-Pentane	n-C5	C5H12
n-Hexane	C6	C6H14
n-Heptane	C7	C7H16
n-Octane	C8	C8H18
n-Nonane	C9	C9H20
n-Decane	C10	C10H22
n-C11	C11	C11H24
n-C12	C12	C12H26
n-C13	C13	C13H28
n-C14	C14	C14H30

Optional Info : PFR-100 @Main -- Unknown Duty

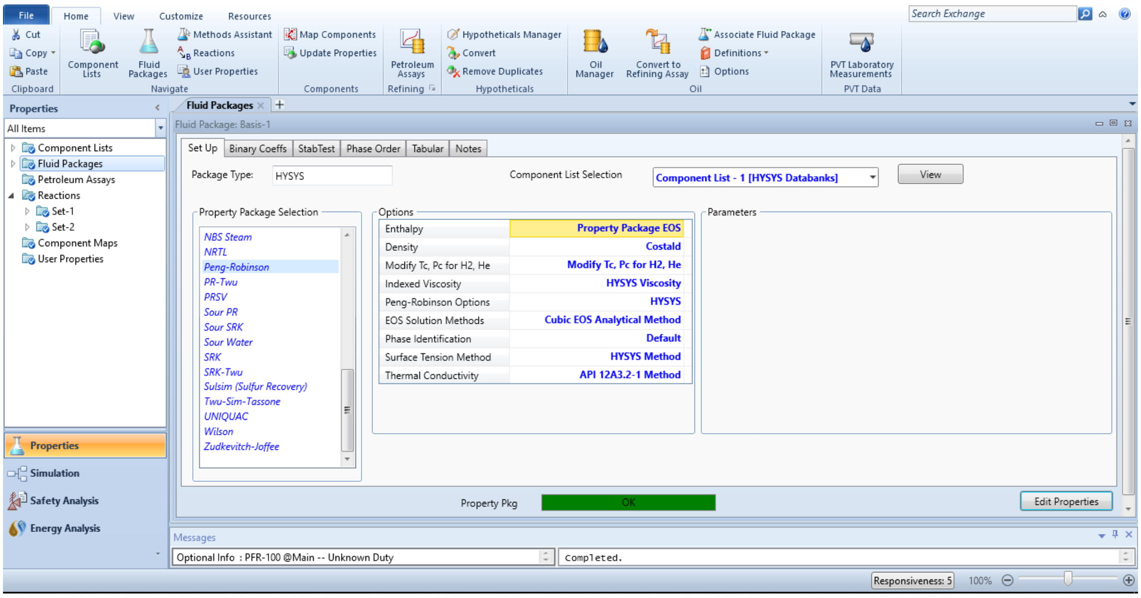
Completed.

Figure 1: Selection of components

2.3.2 Thermodynamic Package Selection

Peng-Robinson property package was used as the equation of state for the modelling because it has been found from the literature that for oil, gas and petrochemical applications, the Peng-Robinson Equation of State is generally the recommended one. To select fluid package,

i. under fluid packages in component list, “add” was clicked and
ii. the Peng Robinson package was selected as seen in Figure 2.



Fluid Package: Basis-1

Package Type: HYSYS

Component List Selection: Component List - 1 [HYSYS Databanks]

Enthalpy	Property Package EOS
Density	Costald
Modify Tc, Pc for H2, He	Modify Tc, Pc for H2, He
Indexed Viscosity	HYSYS Viscosity
Peng-Robinson Options	HYSYS
EOS Solution Methods	Cubic EOS Analytical Method
Phase Identification	Default
Surface Tension Method	HYSYS Method
Thermal Conductivity	API 12A3.2-1 Method

Property Pkg: OK

Optional Info : PFR-100 @Main -- Unknown Duty

```
Completed.
```

Figure 2: Selection of fluid package

2.3.3 Reaction Sets Selection

The reactions involved in the process were inputted in the reaction environment. To select the reactions,

i. under reactions in component list, “add” was clicked,
ii. a reaction set was added as “Set-1’’ and “Add reaction” was clicked.
iii. under the “Add reaction”, HYSYS was selected for reactant source and equilibrium reaction was selected and added,
iv. ‘’Rxn-1” was clicked on and the components involved in the reaction were added,
v. the stoichiometric coefficients for the equation were inputted making those of the reactants to be negative sign and those of the products to be positive,
vi. steps I-V were repeated for all the reactions needed in “Set-1”,
vii. thereafter, “Add to FP” and “Add set to fluid package” were was clicked on successively,
viii. steps I-VI were repeated for “Set-2” with the addition of changing the equilibrium reaction to conversion type in step III,
ix. under step V, the base component was chosen and the percentage conversion (CO) was inputted; then step VII was repeated,
x. steps I-VII were repeated for “Set-3”,
xi. the steps used for “Set-2” were applied for “Set-4”, and
xii. steps I-VII were repeated for “Set-5” with selecting kinetic reaction instead of conversion reaction.

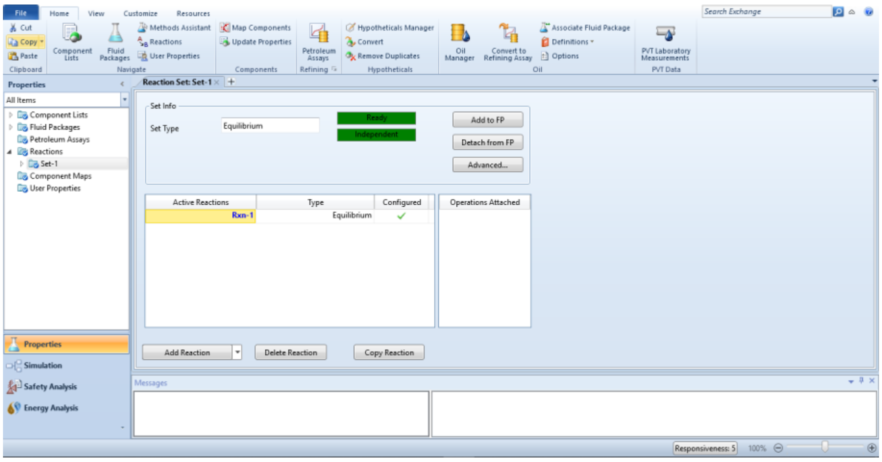
The chemical reactions shown in Equations (1) – (3) were put into Set 1.

$$C_2H_6 + 2H_2O \longrightarrow 2CO + 5H_2 \qquad (1)$$

$$C_3H_8 + 3H_2O \longrightarrow 3CO + 7H_2 \qquad (2)$$

$$C_4H_{10} + 4H_2O \longrightarrow 4CO + 9H_2 \qquad (3)$$

Figure 3 shows the pictorial representation of the selection of Reaction sets in Aspen HYSYS while Figures 4 and 5 shows the interface for selection of reaction set for equilibrium reaction and conversion reaction, respectively.



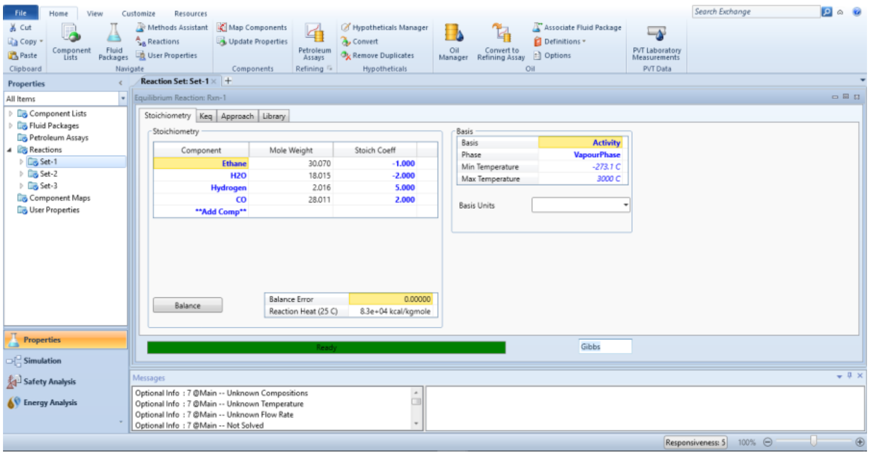
Set Info

Set Type: Equilibrium — Ready — Independent

Active Reactions	Type	Configured
Rxn-1	Equilibrium	✓

Operations Attached

Figure 3: Selection of reaction sets



Stoichiometry

Component	Mole Weight	Stoich Coeff
Ethane	30.070	-1.000
H2O	18.015	-2.000
Hydrogen	2.016	5.000
CO	28.011	2.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	8.3e+04 kcal/kgmole

Basis

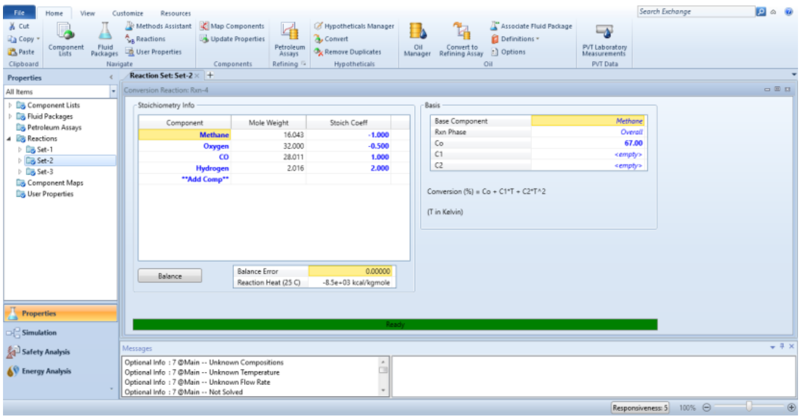
Basis	Activity
Phase	VapourPhase
Min Temperature	-273.1 C
Max Temperature	3000 C

Basis Units

Ready — Gibbs

Optional Info : 7 @Main -- Unknown Compositions
Optional Info : 7 @Main -- Unknown Temperature
Optional Info : 7 @Main -- Unknown Flow Rate
Optional Info : 7 @Main -- Not Solved

Figure 4: Selection of reaction set for equilibrium reaction



Stoichiometry Info

Component	Mole Weight	Stoich Coeff
Methane	16.043	-1.000
Oxygen	32.000	-0.500
CO	28.011	1.000
Hydrogen	2.016	2.000
Add Comp		

Balance Error	0.00000
Reaction Heat (25 C)	-8.5e+03 kcal/kgmole

Basis

Base Component	Methane
Rxn Phase	Overall
Co	67.00
C1	<empty>
C2	<empty>

Conversion (%) = Co + C1*T + C2*T^2

(T in Kelvin)

Ready

Optional Info : 7 @Main -- Unknown Compositions
Optional Info : 7 @Main -- Unknown Temperature
Optional Info : 7 @Main -- Unknown Flow Rate
Optional Info : 7 @Main -- Not Solved

Figure 5: Selection of reaction set for conversion reaction

2.3.4 Flowsheet Development

The process model was built step by step on Aspen HYSYS V11 flowsheet environment using the following approaches. To develop the model of the GTL plant, one distillation column (for the products), two heaters, four reactors (pre-reformer, auto-thermal reformer, water gas shift reactor and Fischer-Tropsch reactor respectively) were inserted on the flowsheet.

Feed

The feed was natural gas containing predominately methane as shown in Table 1. To select this,

(i) under view, model palette was clicked on and the material stream arrow was dragged to the flowsheet environment,
(ii) the material stream was double-clicked and its name was changed to “Feed”.
(iii) the necessary data were entered at the worksheet of the feed as shown in Table 2.
(iv) steps I-III were repeated for the streams named ”Steam” and “Air”.

Table 1: Composition for the feed streams

Component	Mole Fraction (%)
Methane	95.5
Ethane	3
Propane	0.5
n-butane	0.4
Nitrogen	0.6
Water	100
Oxygen	100

Table 2: Inlet conditions and molar flow of the feed streams

Input	Temperature(˚C)	Pressure (bar)	Flowrate (kgmole/h)
Natural gas	40	30	8195
Steam	252	40.45	1400
Oxygen	300	40	4500

Mixer (MIX-101)

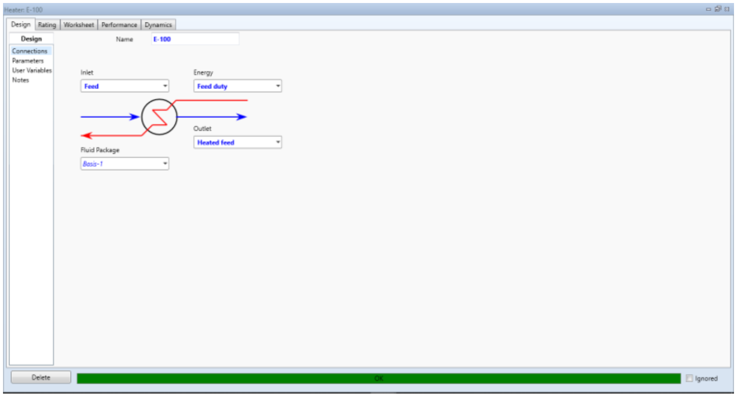
A mixer was installed after the feed stream. It was used to join the feed and recycle stream before being sent to the heater. To achieve this,

i. the mixer was selected from the model palette.
ii. it was double-clicked on to access its tabs (design, connections), and
iii. "Feed” was selected as the inlet stream and the outlet stream named “Mixed feed” was created; the “Recycle” stream was later added to the inlet stream of the mixer (Figures 6 and 7).

Heater (E-100)

A heater was installed to raise the temperature of the feed from 40 ˚C to 675 ˚C. To accomplish this,

(i) the heater was selected from the model palette,
(ii) it was double-clicked on to access its connections under design,
(iii) "Mixed feed" was selected as the inlet stream and the outlet stream was named as "Heated feed" while the energy stream was denoted as "Feed duty",
(iv) in parameters, 0 bar was entered as delta P, and
(v) under worksheet, going to conditions, the data for the outlet stream temperature were inputted.



Name: E-100
Inlet: Feed
Energy: Feed duty
Outlet: Heated feed
Fluid Package: Basis-1

Figure 6: Installation of the heater

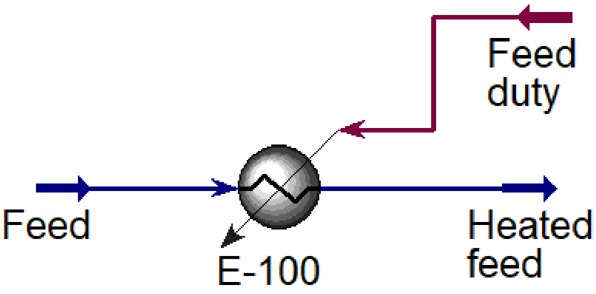


Figure 7: Heater

Pre-reformer (CRV 100 & ERV 100)

The Pre-reformer was modelled as a conversion reactor. The reactant streams were feed and steam, whereas the water gas shift reactors were modelled as an equilibrium reactor. For the Pre-reformer, the conversion reactor was selected from the model palette and connected as shown in Figure 8. Thereafter, the equilibrium reactor was selected from the Model Palette of the Aspen HYSYS and connected (see Figures 9 and 10). The data for the reactions occurring in the pre-reformer are given in Table 3.

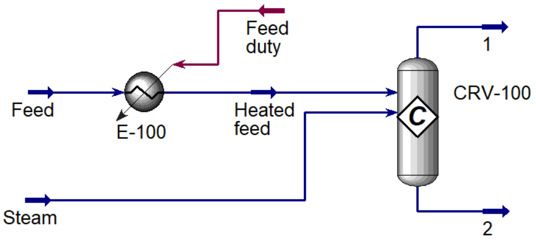
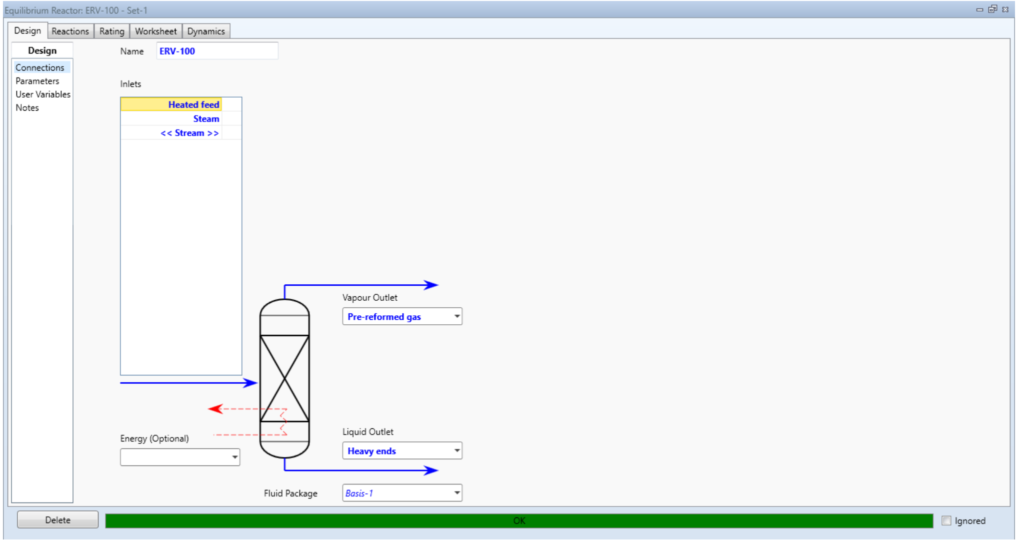


Figure 8: Pre-reformer conversion reactor


Equilibrium Reactor: ERV-100 - Set-1

Name ERV-100

Inlets
Heated feed
Steam
<< Stream >>

Vapour Outlet: Pre-reformed gas

Liquid Outlet: Heavy ends

Energy (Optional):

Fluid Package: Basis-1

OK

☐ Ignored

Figure 9: Installation of the Pre-reformer equilibrium reactor

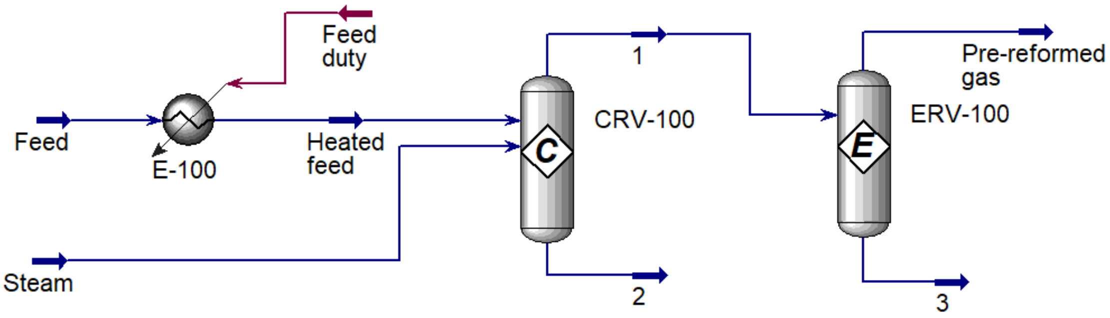


Figure 10: Pre-reformer conversion reactor

Table 3: Reactions in the pre-reformer and their corresponding enthalpy of reactions

Reaction	$\Delta_{rxn}H^{\circ}_{298}$[kJ/mol]
$C_2H_6 + 2H_2O \longrightarrow 2CO + 5H_2$	350
$C_3H_8 + 3H_2O \longrightarrow 3CO + 7H_2$	500
$C_4H_{10} + 4H_2O \longrightarrow 4CO + 9H_2$	650
$CO + 3H_2 \rightleftharpoons CH_4 + H_2O$	-210
$CO + H_2O \rightleftharpoons CO + H_2$	-41

Heater (E-101)

A heater was installed to raise the temperature of the pre-reformed gas from 500 ˚C to 800 ˚C prior to its being fed into the auto-thermal reforming (ATR) unit. To achieve this, the heater was selected from the Model Palette, the necessary input and output streams were attached, and appropriate data were entered for the simulation as shown in Figure 11.

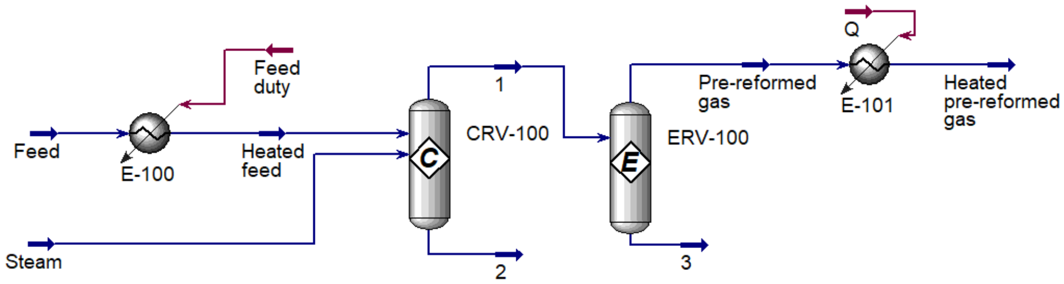


Figure 11: Installation of heater downstream of pre-reformer

Reformer (CRV 101 & ERV 101)

The Autothermal Reformer (ATR) was modelled as a conversion reactor, as combined in Figure 12. The ATR combines the thermal effects of the exothermic POR and endothermic SR by feeding the natural gas, air and water into the reactor. Here, most of the methane was converted to carbon monoxide and hydrogen. The air was modelled as a pure oxygen stream entering at 200 ˚C. After the Auto-thermal reaction, water gas shift reaction (WGSR) and the CO_2 reforming reaction occurred. The CO_2 from the WGSR was consumed to form more synthesis gas. The water gas shift reactors are modelled using as an equilibrium reactor, as shown in Figure 13.

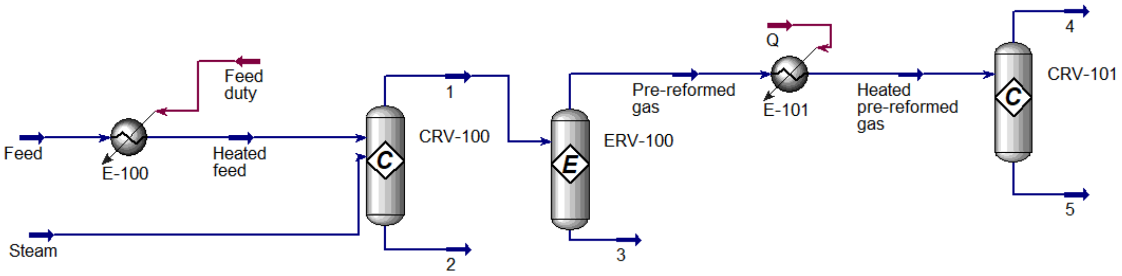


Figure 12: Reformer conversion reactor combined

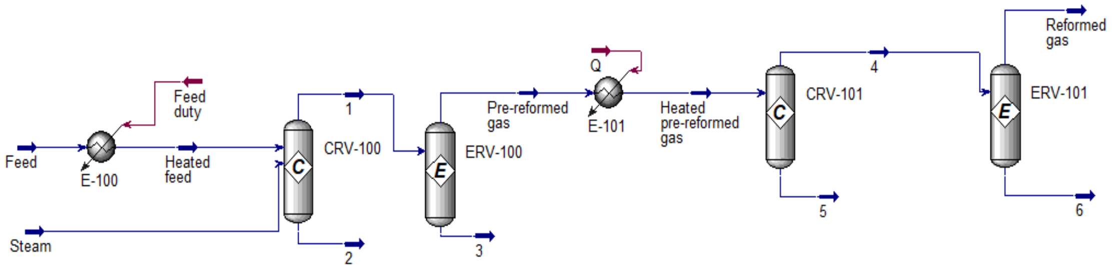


Figure 13: Reformer equilibrium reactor combined

The reactions occurring in the reformer and the corresponding enthalpy of the reactions are given in Table 4.

Table 4: Reactions in the reformer and their corresponding enthalpy of reactions

Reaction	$\Delta_{rxn}H^{\circ}_{298}$ [kJ/mol]
$CH_4 + \frac{1}{2}O_2 \longrightarrow CO + 2H_2$	-44

$CH_4 + H_2O \rightleftharpoons CO + 3H_2$	206
$CO + H_2O \rightleftharpoons CO + H_2$	-41

Cooler (E-102)

A waste heat boiler is usually used after the ATR to lower the temperature of the syngas, but for simplicity, in this case, it was modelled as a cooler (Figure 14).

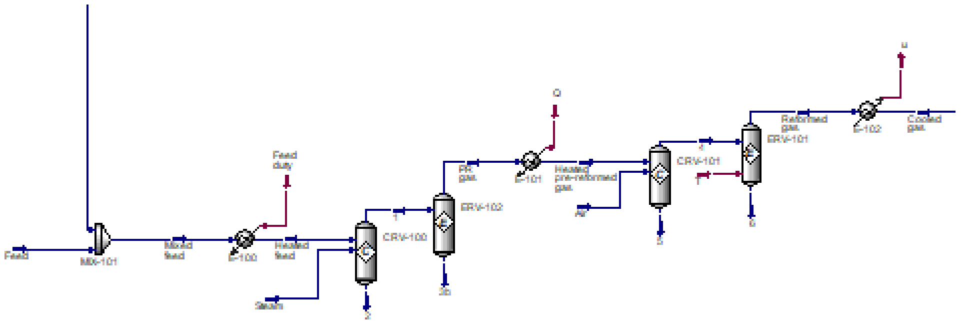


Figure 14: Combination of cooler to the installation

Thereafter, a Separator (V-101) that was used to separate the excess water from the cooling process prior to the gas being mixed with the recycle gas was included as a two-phase separator, a Mixer (MIX-100) connecting the syngas and the recycled gas, a Recycle block (RCY-1), a Heater (E-103) that was used to raise the temperature of the cooled gas from 38 ˚C to 210 ˚C before it was fed to the FT reactor were connected to obtain the flow diagram given in Figure 15.

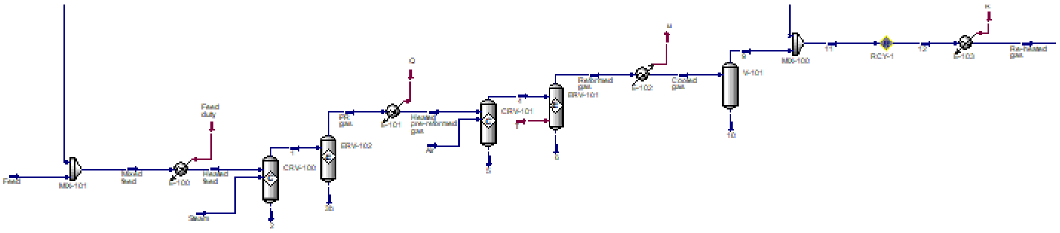


Figure 15: Heater-combined flowsheet

Fischer-Tropsch Reactor (PFR-100)

A multi tubular fixed bed was used as FTR and modelled as a plug flow reactor (Figure 16). The Low Temperature Fischer-Tropsch (LTFT) reactor was used for the process and a multi tubular flow reactor was employed. The LTFT was used in the production of wax and for the purpose of utilising stranded gas. The temperature range for this operation was between 200-240 ˚C.

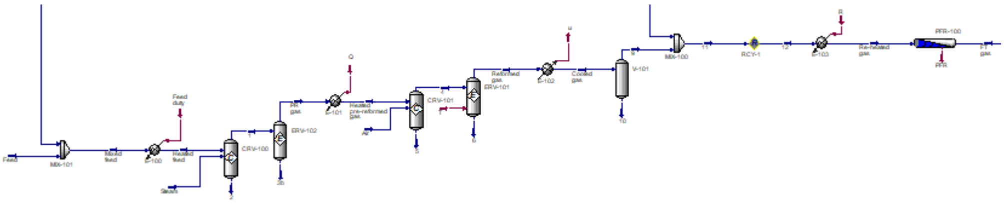


Figure 16: Installation of FT reactor

The kinetics chosen for the modeling of the Fischer-Tropsch reactions in this work was the one given by Iglesia *et al.* (1993) for a cobalt catalyst. They proposed the reaction rates for methane production and CO consumption on a cobalt catalyst were as shown in Equations (4) and (5). The reaction rates were obtained to be valid at 473-483 K, 100-3000 kPa, H_2/CO = 1–10, and CO conversions lower than 15% (Rafiee and Panahi, 2016). Other parameters for the process are given in Tables 5 – 7.

$$r_{CH4} = \frac{k_1 P_{H_2} {P_{CO}}^{0.05}}{1 + k_1 P_{CO}} \tag{4}$$

$$r_{CO} = \frac{k_2 {P_{H_2}}^{0.6} {P_{CO}}^{0.65}}{1 + k_1 P_{CO}} \tag{5}$$

Table 5: Reactions modelled in the Fischer-Tropsch reactor and their corresponding enthalpy of reactions

Reaction	$\Delta_{rxn}H^{\circ}_{298}$[kJ/mol]
$CO + 2.1H_2 \rightarrow \sum_{i=1}^{20} (ASF\ Coefficeint)_i\, C_iH_{2i+2} + (ASF\ Coefficeint)_{30} C_{30}H_{62} + H_2O$	-160
$CH_4 + H_2O \rightleftharpoons CO + 3H_2$	-210

Table 6: Kinetic and adsorption parameters for modelling the Fischer-Tropsch reactions

Parameter	**Arrhenius expression**
K_1[kmol$_{CH4}$Pa$^{-1.05}$ m^{-3}$_{reactor}$s^{-1}]	$8.8 \times 10^{-6} \quad \exp(-\frac{37326}{RT})$
K_1[Pa^{-1}]	$1.096 \times 10^{-12} \quad \exp(-\frac{-68401.5}{RT})$
K_1[kmol$_{CO}$Pa$^{-1.25}$ m^{-3}$_{reactor}$s^{-1}]	$1{,}6 \times 10^{-5} \quad \exp(-\frac{37326}{RT})$

Table 7: Parameters in the Fischer-Tropsch reactor

Temperature (˚C)	Volume (m^3)
210	1000

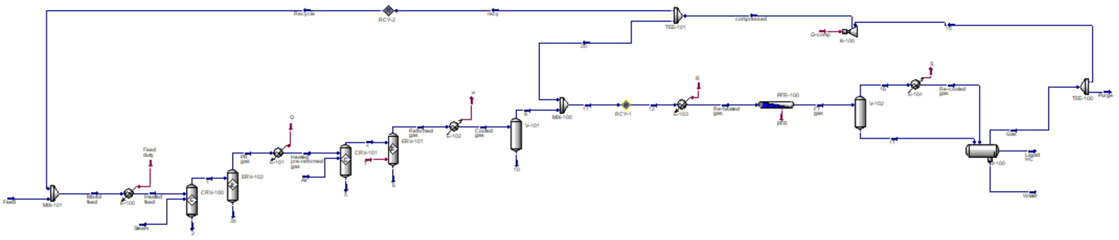


Figure 17: Final flowsheet

After the Fischer-Tropsch reactor, a Separator (V-102), which was used to separate the excess water from the cooling process prior to the gas being mixed with the recycle gas, a Cooler (E-104) used to cool the gas to 38 ˚C by exchanging the excess heat with water before being sent to the separator, another Separator (V-100) used to separate the gas from the liquid before it was sent to the upgrading unit, a Tee (TEE-100) for connecting the syngas and the recycled gas, a Compressor (K-100) used to increase the pressure of the gas before it was sent as a recycle to the join the feed, another Tee (TEE-101) and another Recycle (RCY-2) were added to the flowsheet to give the final form shown in Figure 17.

3. Results and Discussion

3.1 Simulation result

Fischer-Tropsch Reactor (FTR) Volume

A case study was conducted using reactor volumes between 400-2400 m^3 in order to investigate how the volume of the reactor affects the molar flow rates of carbon monoxide and hydrogen obtained from the process.

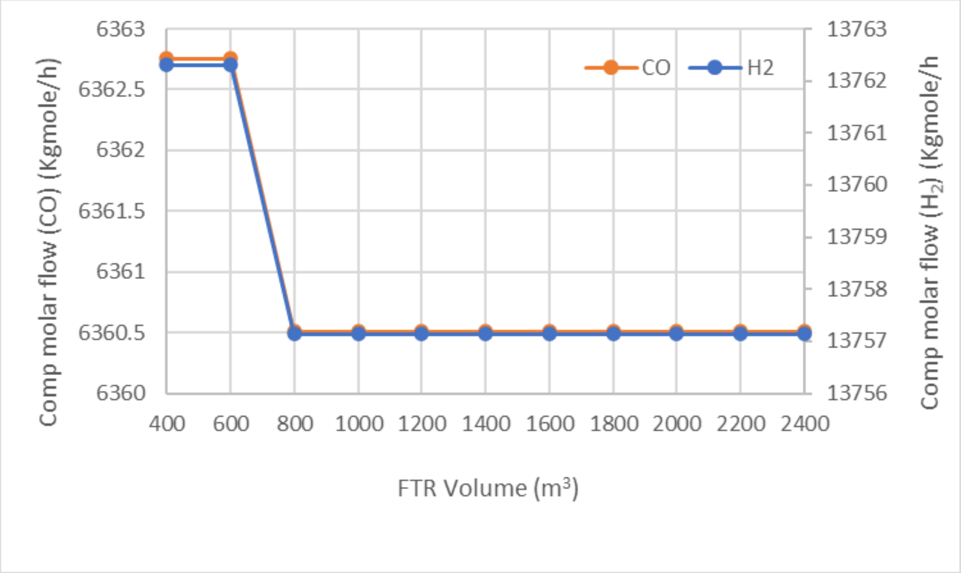


Figure 18: Plot of molar flow of hydrogen and carbon monoxide (kmol/h) as a function of FTR volume (m^3).

According to the results shown in Figure 18, the molar flow of CO and H_2 were found to be affected by the volume of the FTR considered. respectively as a function of the reactor volume for the base case. It was also observed from the results given in the figure that the molar flow rate of the carbon monoxide and that of the hydrogen became constant as from the reactor volume of 800 m^3.

Molar flow of Oxygen

A case study was as well conducted using molar flow rates of oxygen between 1000-5000 kgmole/h. The results obtained from this investigation are given in Figures 19 – 21. The figures show how the temperature of the syngas, H_2/CO ratio from the ATR and the flowrate of the products to the upgrading unit is affected by oxygen, respectively.

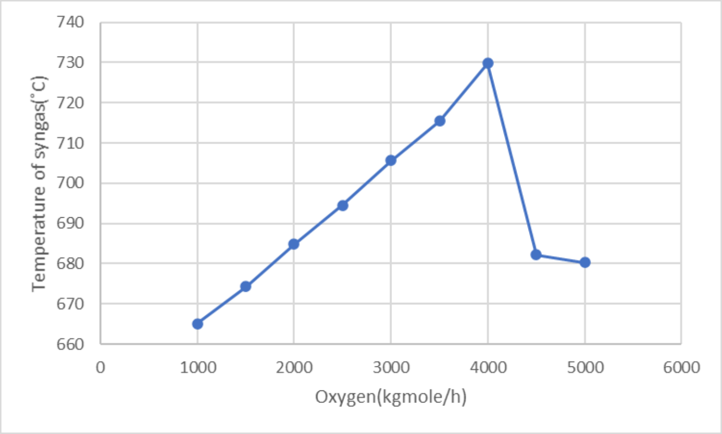


Figure 19: Plot of temperature of syngas as a function of molar flow of oxygen in the range 1000-5000 kgmole/h

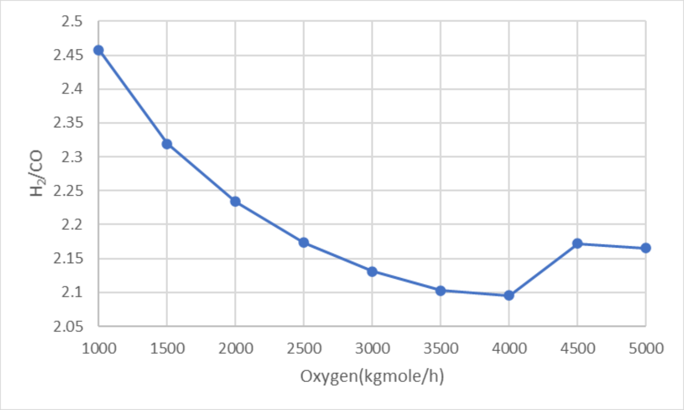


Figure 20: Plot of H_2/CO ratio in the syngas leaving the ATR as a function of molar flow of oxygen in the range 1000-5000 kgmol/h

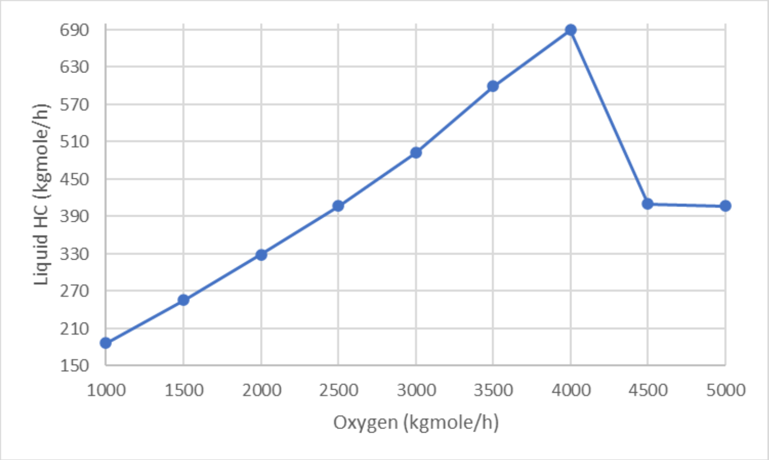


Figure 21: Plot of molar flowrate of liquid HC as a function of molar flow of oxygen in the range 1000-5000 kgmol/h

From the results shown Figure 19, it was discovered that the temperature was increasing with increase in molar flow of oxygen till it exceeded a molar flow of 4000 kgmole/h. The highest temperature of 730 ˚C was also observed to occur at 4000 kgmole/h. This temperature was found acceptable as it did not exceed a soot formation temperature of 1030 ˚C. From Figure 20, it can be observed that a H_2/CO ratio of 2.16 was achieved at a flowrate of 4500 kgmole/h. The exact ratio of 2.1 was gotten at 3000 kgmole/h and can be achieved through optimization of the model. According to the results shown in Figure 21, it was seen that as the molar flow of oxygen was increasing, the molar flow of products was also increasing. However, at a point, an increase in the flowrate was found to lead to a decrease in the flow of the products. From the graph, it can be seen that the flowrate that gave the maximum product flowrate was 4000 kgmole/h.

Molar flow of Steam

A case study was conducted using molar flow rates of steam between 1000-5000 kgmole/h. Figures 22 – 24 are the results obtained from the study of how the temperature of the syngas gas, H_2/CO ratio from the ATR and the flowrate of the products to the upgrading unit is affected by steam.

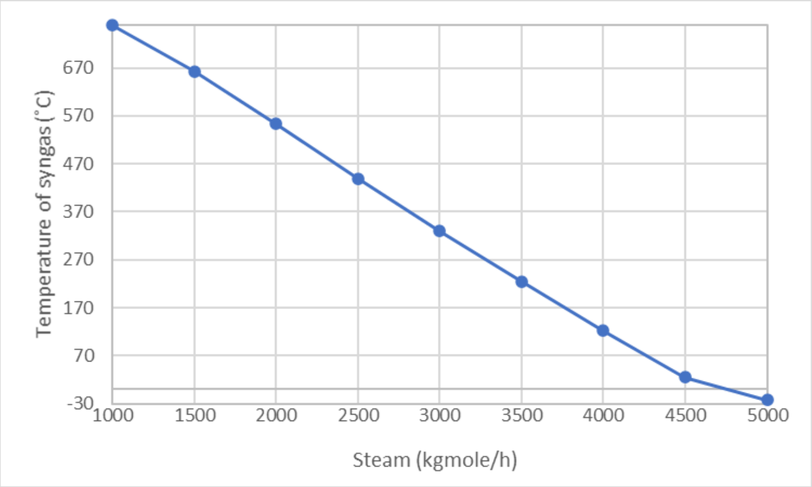


Figure 22: Plot of temperature of syngas as a function of steam in the range of 1000-5000 kgmole/h

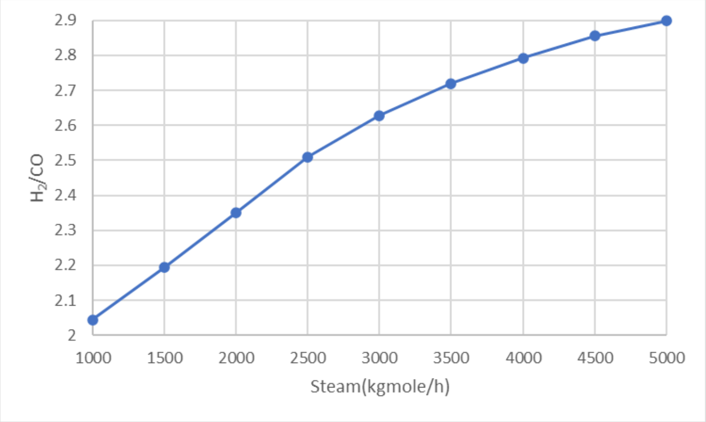


Figure 23: Plot of Plot of H_2/CO ratio in the syngas leaving the ATR as a function of molar flow of steam in the range 1000-5000 kgmole/h

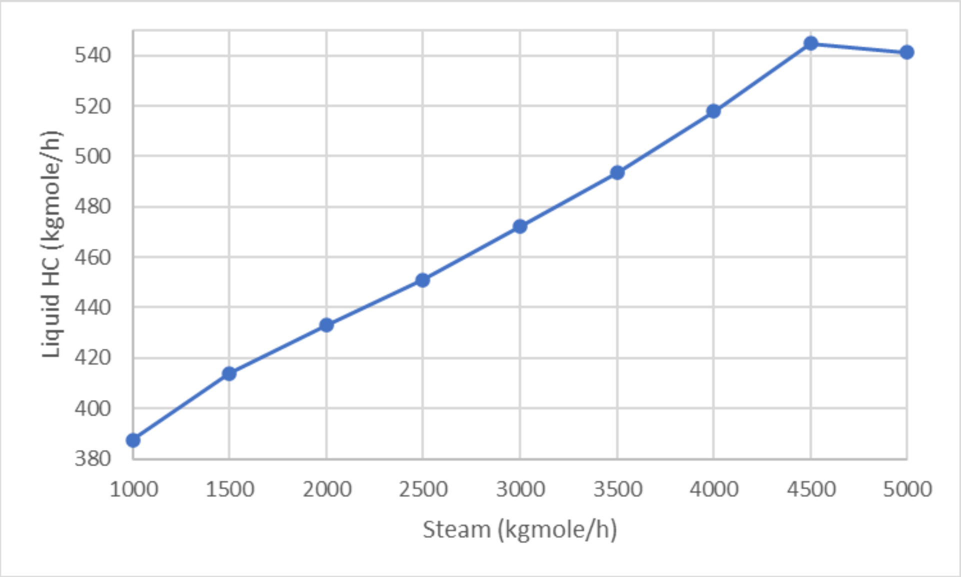


Figure 24: Plot of Plot of molar flowrate of liquid HC as a function of molar flow of steam in the range 1000-7000 kgmole/h

Based on the results given in Figure 22, the temperature was found to decrease with increase in molar flow of steam. In order to keep the temperature of the syngas at a reasonable level, the molar flow of steam had to be below 5000 kgmole/h. From Figure 23, it was observed that, to keep the H_2/CO ratio at approximately 2.1, the molar flow of oxygen had to be below 1500 kgmole/h. Increasing the molar flow would shift the H_2/CO ratio higher to an undesired value. From Figure 24, it was seen that as the molar flow of oxygen was increasing, the molar flow of products was also increasing. However, an increase in the flowrate was found to lead to a decrease in the flow of products at a particular point. According to the graph, a steam flowrate of 4500 kgmole/h gave the maximum product flowrate. However, for the purpose of maintaining of H_2/CO ratio of 2.1, a steam flow of 1400 kgmole/h was used despite the fact that it would result in a lower flow of products.

3.2 Analysis of the simulation

Taking a look at the stream leaving the pre-reformer (PR gas), it could be seen that the higher hydrocarbons were used up in the reaction, which was an indication of good operation in the unit. In addition, looking at the reformed gas stream, it was observed that most of the higher hydrocarbons were used up and a H_2/CO ratio value of 2.16 was achieved, which was found to be close to the theoretical value of 2.1. Also, it was observed that the CO was used up and the amount of H_2 that was present in stream leaving the reactor (FT gas) was minimal and indicating good conversion in the reactor. Moreover, the liquid hydrocarbon stream going to the upgrading unit consisted of hydrocarbons that can be used to manufacture desired products such as gasoline, kerosene, diesel and wax with small amounts of liquefied petroleum gas, methane and hydrogen. This was found to be an indication of an effective separation occurring after the reaction.

4. Conclusion

The results obtained from the simulation carried out in this work showed that a model of a gas-to-liquid (GTL) plant using the Fischer-Tropsch process has been successfully developed and simulated with the aid of Aspen HYSYS. This study has provided a base case for the simulation of a GTL plant using an autothermal reforming technology for the production of synthesis gas and a multi-tubular reactor for the low temperature Fischer Tropsch reactor. The parameter study conducted using case studies gave good insights into how the variables relate. It was discovered from the study that natural gas was converted to liquid hydrocarbons, which can be further processed to produce other liquid products.

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